

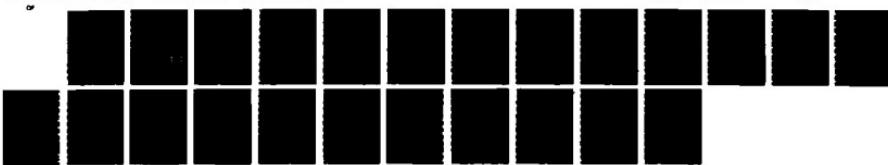
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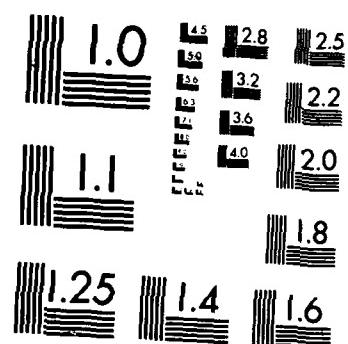
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RELAXATION FUNCTIONS, MEMORY FUNCTIONS, RANDOM FORCES, AND ERGODICITY  
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by

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RELAXATION FUNCTIONS, MEMORY FUNCTIONS, RANDOM FORCES, AND ERGODICITY  
IN THE ONE-DIMENSIONAL SPIN- $\frac{1}{2}$  XY AND TRANSVERSE ISING MODELS

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→ Tr. Document  $\langle S_x \rangle_{over j}$ .  
We investigate the dynamics of the one-dimensional  $S=\frac{1}{2}$  isotropic XY model and transverse Ising model in the high temperature limit by using the method of recurrence relations. We obtain the relaxation functions as well as some Brownian analogs of a generalized Langevin equation for a tagged spin  $S_j^x$  in these models, namely, the memory functions and the random forces. It is found We find that the realized dynamical Hilbert spaces of the two models have the same structure, which leads to similar dynamical behavior apart from a time scale. Based on the infinite dimensionality of these Hilbert spaces we also concluded that  $S_j^x$  is ergodic in both models. ←

$\langle X \rangle_{over j}$



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## I. INTRODUCTION

The one-dimensional spin- $\frac{1}{2}$  XY model has been of considerable theoretical interest in recent years as a solvable many-body system<sup>1</sup>. The Hamiltonian of this model is given by

$$H = 2 \sum_i^N (J^x S_i^x S_{i+1}^x + J^y S_i^y S_{i+1}^y) - B \sum_i^N S_i^z, \quad (1.1)$$

where  $S_i^\alpha$  are spin operators,  $J^\alpha$  are the coupling constants, and  $B$  is an external magnetic field. Periodic boundary conditions are imposed, so that  $S_{N+1}^\alpha = S_1^\alpha$ , where  $N$  is the total number of spins and  $\alpha = x, y, \text{or } z$ . In this paper we are concerned with two particular cases of this Hamiltonian, namely, the isotropic XY model (XY) for which  $J^x = J^y = J$ ,  $B = 0$ , and the transverse Ising model (TI) where  $J^x = J$ ,  $J^y = 0$ , and  $B = J$ .

Although the equilibrium properties of these systems are well known<sup>1,2</sup>, their dynamical behavior is less well understood. There are exact results for the longitudinal time-dependent spin correlation functions due to Niemeijer<sup>3</sup>, and for the transverse correlation functions in the limit of high temperature obtained by Brandt and Jacoby<sup>4</sup> and also by Capel and Perk<sup>5</sup>. The transverse spin correlation functions for both the XY and TI cases in the high temperature limit are found to be

$$\langle S_j^x(t) S_j^x \rangle = \frac{1}{4} e^{-\Delta t^2}, \quad (1.2)$$

where  $\Delta = J^2$  for the XY case, and  $J^2/2$  for the TI case. The underlying reason why the two cases have the same time dependence has not been recognized so far.

In this paper we use the method of recurrence relations due to Lee<sup>6</sup> to study the time evolution of both the isotropic XY model and the transverse Ising model in the high temperature limit. This method allows one to obtain a detailed yet rigorous description of the dynamics in such systems. It has been applied to some spin models<sup>7</sup>, to an electron gas<sup>8</sup>, to a classical harmonic oscillator chain<sup>9</sup>, and to the study of velocity autocorrelation functions<sup>10</sup>.

In the method of recurrence relations the time evolution of a dynamical variable, e.g.  $S_j^X(t)$ , is described as an orthogonal expansion in a properly defined Hilbert space, where the time dependency is placed on the expansions coefficients. By inspecting the relative norms of the dynamical Hilbert space for each of the XY and TI cases we can readily see why these systems are dynamically equivalent in the high temperature limit. With relatively little effort we recover the transverse correlation function (1.2) for these systems. We would also like to point out that these systems are dynamically equivalent to the spin Van der Waals model studied by Lee, Kim, and Dekeyser<sup>7</sup>. We conjecture that there may also be other systems with similar dynamical behavior, for which their respective dynamical Hilbert spaces have the same geometry, that is, the same dimensionality and also the same relative norms of basis vectors.

To obtain further insight in the time evolution of these systems we calculate some Brownian analogs of a generalized Langevin equation for the spin variables, namely, the spin memory function and the spin random force. We also discuss ergodicity in these models based on the dimensionality of the realized Hilbert spaces of the dynamical variables of interest.

The arrangement of this paper is as follows. In Sec. II we review the method of recurrence relations as well as its connections to a generalized Langevin equation. In Sec. III that method is applied to the dynamical behavior of the isotropic XY model and the transverse Ising model. Correlation functions, relaxation functions, memory functions, and random forces are then obtained. Finally, in Sec. IV we summarize our results and discuss ergodicity in these systems.

## II. METHOD OF RECURRENCE RELATIONS

Consider a one-dimensional  $N$  spin- $\frac{1}{2}$  system described by a Hamiltonian  $H$ . The time evolution of an operator  $G$  is given formally by

$$G(t) = e^{itL} G(0), \quad (2.1)$$

where  $L$  is the Liouville operator for the system, defined by

$$iLf \equiv [f, H] \equiv fH - Hf. \quad (2.2)$$

Equation (2.1) can also be expressed by the expansion<sup>6</sup>

$$G(t) = \sum_{v=0}^{d-1} a_v(t) f_v, \quad (2.3)$$

where  $f_v$  are basis vectors of a Hilbert space  $\mathcal{H}$  of  $d$  dimensions. The positive definite scalar product in  $\mathcal{H}$  is defined in the high temperature limit ( $T=\infty$ ) as

$$(A, B) \equiv \frac{1}{Z} \text{Tr } AB^+ \quad (2.4)$$

where  $Z = 2^N$  is the partition function of the system in this limit.

By choosing  $f_0 \equiv G(0)$  it follows that the remaining basis vectors  $f_v$  can be generated by the following recurrence relation (RRI):

$$f_{v+1} = iLf_v + \Delta_v f_{v-1}, \quad v \geq 0, \quad (2.5)$$

where

$$\Delta_v = \frac{(f_v, f_v)}{(f_{v-1}, f_{v-1})}, \quad v \geq 1, \quad (2.6)$$

are the relative norms of the basis vectors, and by definition

$$f_{-1} \equiv 0, \Delta_0 \equiv 1.$$

The coefficients  $a_v(t)$ , which are also the relaxation functions, satisfy a second recurrence relation (RRII):

$$\dot{a}_{v+1} a_{v+1}(t) = -\dot{a}_v(t) + a_{v-1}(t), \quad v \geq 0, \quad (2.7)$$

where  $\dot{a}_v(t) \equiv \frac{da_v(t)}{dt}$ ,  $a_{-1} \equiv 0$ . Notice that due to the initial choice  $f_0 = G(0)$ , it follows from Eq.(2.3) that  $a_0(0) = 1$ , and  $a_v(0) = 0$  for  $v \geq 1$ . The complete time evolution of  $G(t)$  can thus be determined by using RRI and RRII.

A generalized Langevin equation for the operator  $G(t)$ , which is formally equivalent to the Heisenberg equation of motion, is given by

$$\frac{dG(t)}{dt} + \int_0^t dt' \phi(t-t') G(t') = F(t), \quad (2.8)$$

where  $\phi$  is the memory function and  $F$  the random force. Both  $\phi$  and  $F$  can be readily obtained as follows. The random force is given by

$$F(t) = \sum_{v=1}^{d-1} b_v(t) f_v, \quad (2.9)$$

where the coefficients  $b_v(t)$  satisfy the convolution equations

$$a_v(t) = \int_0^t dt' b_v(t-t') a_0(t'), \quad v \geq 1. \quad (2.10)$$

The memory function is given simply by  $\phi(t) = b_1(t)$ . The remaining  $b_v$ 's, that is,  $b_2, b_3, \dots$ , are the 2nd memory function, 3rd memory function, ..., etc. The reader is referred to the original formulation of the method of recurrence relations for the detailed derivations of the relations contained in this section<sup>6</sup>.

### III. DYNAMICS OF THE XY AND TI MODELS

In this section we apply the method of recurrence relations described in Sec. II to investigate the dynamical properties of the XY and TI models at  $T = \infty$ . Consider first the XY case, taking  $S_j^X$  as the dynamical variable of interest. The time evolution of  $S_j^X(t)$  is given, according to Eq.(2.3), as

$$S_j^X(t) = \sum_{v=0}^{d-1} a_v(t) f_v, \quad (3.1)$$

where  $f_0 = S_j^X(0) = S_j^X$ . By using RRI we obtain

$$f_1 = 2J(S_{j-1}^y S_j^z + S_j^z S_{j+1}^y),$$

$$f_2 = -4J^2(S_{j-2}^x S_{j-1}^z S_j^z - S_{j-1}^x S_j^y S_{j+1}^y + 2S_{j-1}^y S_j^x S_{j+1}^y - S_{j-1}^y S_j^y S_{j+1}^x + S_j^z S_{j+1}^z S_{j+2}^x),$$

$$\begin{aligned} f_3 = & 2J^3(-4S_{j-3}^y S_{j-2}^z S_{j-1}^z S_j^z + 4S_{j-2}^y S_{j-1}^z S_j^y S_{j+1}^y - 8S_{j-2}^x S_{j-1}^z S_j^y S_{j+1}^x \\ & + 12S_{j-2}^x S_{j-1}^z S_j^x S_{j+1}^y + 3S_{j-1}^y S_j^z + 3S_{j-1}^z S_j^y + 12S_{j-1}^y S_j^x S_{j+1}^z S_{j+2}^x) \end{aligned}$$

$$- 8S_{j-1}^x S_j^y S_{j+1}^z S_{j+2}^x + 4S_{j-1}^y S_j^y S_{j+1}^z S_{j+2}^y - 4S_j^z S_{j+1}^z S_{j+2}^z S_{j+3}^y),$$

$$f_4 = 8J^4\{S_{j-2}^x S_{j-1}^x S_{j+1}^x + S_{j-1}^x S_{j+1}^x S_{j+2}^x - 2(S_{j-2}^y S_{j-1}^x S_{j+1}^y + S_{j-1}^y S_{j+1}^x S_{j+2}^y) \\ - S_{j-4}^x S_{j-3}^z S_{j-2}^z S_{j-1}^z S_j^z + S_{j-3}^x S_{j-2}^z S_{j-1}^z S_j^y S_{j+1}^y + S_{j-1}^y S_j^y S_{j+1}^z S_{j+2}^z S_{j+3}^x$$

$$- S_{j-1}^z S_{j+1}^z S_{j+2}^z S_{j+3}^z S_{j+4}^x) + 3(S_{j-2}^x S_{j-1}^y S_{j+1}^x + S_{j-1}^y S_{j+1}^y S_{j+2}^x - S_{j-1}^z S_j^x S_{j+1}^z) \\ - 4(S_{j-2}^x S_{j-1}^z S_{j+1}^z + S_{j-1}^z S_{j+1}^z S_{j+2}^z) - 6(S_{j-3}^y S_{j-2}^z S_{j-1}^z S_j^y S_{j+1}^x) \\ + S_{j-2}^x S_{j-1}^z S_j^y S_{j+1}^z S_{j+2}^y + S_{j-2}^y S_{j-1}^z S_j^y S_{j+1}^z S_{j+2}^x + S_{j-1}^x S_j^y S_{j+1}^z S_{j+2}^z S_{j+3}^y)\}$$

$$+ 8(s_{j-3}^y s_{j-2}^z s_{j-1}^z s_j^x s_{j+1}^y + s_{j-1}^y s_j^x s_{j+1}^z s_{j+2}^z s_{j+3}^y) - 12s_{j-2}^x s_{j-1}^z s_j^x s_{j+1}^z s_{j+2}^x \},$$

etc. (3.2)

Thus an excitation of  $s_j^x$  at  $t=0$  will propagate through the chain according to Eqs.(3.1 and 2). The basis vectors  $f_v$  correspond to excitations of clusters of spin. There is a spatial hierarchy in the  $f_v$ 's in the sense that as  $v$  increases, so do the boundaries of the region in the chain within which clusters of spins are excited. As we shall see later, there is also a hierarchy in the time sequence in which the vectors  $f_v$  are excited, so that a true propagation of the initial excitation throughout the chain does indeed take place. In addition, the length of the clusters generally increases with  $v$ . Notice also the appearance of "disconnected" clusters in vectors  $f_v$  of higher dimensions of  $\mathcal{H}$  consisting of groups of spins in which at least one of the spins is separated from the others, e.g.  $s_{j-2} s_{j-1} s_{j+1}$  in  $f_4$ .

The relative norms  $\Delta_v$  are easily obtained from Eqs.(2.4,6) and (3.2). We find  $\Delta_1 = \Delta$ ,  $\Delta_2 = 2\Delta$ ,  $\Delta_3 = 3\Delta$ , etc., where  $\Delta = 2J^2$ . The quantity  $\Delta^{1/2}$  is referred to in the literature as the basal frequency<sup>7</sup>. In the thermodynamic limit there is no upper bound for  $v$ , so that the dynamical Hilbert space  $\mathcal{H}$  has infinite dimensions ( $d = \infty$ ), and the relative norms are given by

$$\Delta_v = v\Delta, \quad v = 1, 2, 3, \dots \quad (3.3)$$

A relation similar to this was also obtained by Lee, Kim, and Dekeyser in their study of the dynamics of the spin Van der Waals model.<sup>7</sup>

The recurrence relation (2.8) now reads

$$(v+1)\Delta a_{v+1}(t) = -\dot{a}_v(t) + a_{v-1}(t), \quad v = 0, 1, 2, \dots \quad (3.4)$$

It is satisfied by

$$a_v(t) = \frac{t^v}{v!} \exp(-\frac{1}{2}\Delta t^2). \quad (3.5)$$

These are the so-called relaxation functions.

In terms of normalized basis vectors  $F_v = (f_v, f_v)^{-\frac{1}{2}} f_v$ ,  
the time evolution of  $S_j^X(t)$  is given by

$$S_j^X(t) = \sum_{v=0}^{\infty} A_v(t) F_v, \quad (3.6)$$

where

$$A_v(t) = \frac{1}{2} \frac{(\frac{1}{2}t)^v}{(v!)^{\frac{1}{2}}} \exp(-\frac{1}{2}\Delta t^2). \quad (3.7)$$

This quantity satisfies the Bessel equality

$$\sum_{v=0}^{\infty} A_v^2(t) = \frac{1}{4}. \quad (3.8)$$

That is, the length of the vector  $S_j^X(t)$  in the dynamical Hilbert space is an invariant of time.<sup>6,10</sup> In Fig.1 we show the time dependent probabilities  $A_v^2(t)$  (normalized to  $\frac{1}{4}$ ) in early stages where  $S_j^X(t)$  samples the space of the lower basis vectors. Notice that due to the pre-exponential factor in  $A_v(t)$ , the basis vectors corresponding to the lower dimensions of  $\mathcal{H}$  are more likely to be initially excited before those of higher dimensions. In addition, each of the

probabilities  $A_v^2(t)$  decay in a Gaussian manner, so that a somewhat localized, yet spreading, group of basis vectors are being excited as time progresses. This corresponds to a propagation of the initial excitation throughout the spin system. This propagation, however, is to be understood in a quantum mechanical context, since the Bessel equality (3.8) holds for all times. That is because actually all the  $f_v$ 's are excited for  $t > 0$  due to the instantaneous nature of the coupling constant. However, at any given  $t$  the probability of excitation is significant only for a fraction of the  $f_v$ 's. On the other hand, it can be seen from Eq.(3.1) that the maxima of the amplitudes  $A_v^2(t)$  are located at  $v = \Delta t^2$ . In the spin chain, that corresponds to the boundaries  $j \pm v$  of the region in which the significant excitations are taking place.

The transverse correlation function can now be obtained as follows:

$$\begin{aligned} \langle S_j^X(t) S_j^X(0) \rangle &= (S_j^X(t), S_j^X) = \frac{1}{4} a_0(t) \\ &= \frac{1}{4} \exp(-\frac{1}{2}\Delta t^2) \\ &= \frac{1}{4} \exp(-J^2 t^2) , \end{aligned} \quad (3.9)$$

which agrees with the results found in the literature.<sup>4,5</sup>

Consider now the TI case. The time evolution of the operator  $S_j^X$  is represented by

$$S_j^X(t) = \sum_{v=0}^{d-1} a'_v(t) f'_v , \quad (3.10)$$

where  $f'_0 = S_j^X(0) = S_j^X$ , and primed variables are used to distinguish the notation here from that of the XY case. By using RRI we obtain

$$\begin{aligned} f'_1 &= JS_j^Y, \\ f'_2 &= -2J^2(S_{j-1}^X S_j^Z + S_j^Z S_{j+1}^X), \\ f'_3 &= -2J^3(S_{j-1}^Y S_j^Z + 4S_{j-1}^X S_j^Y S_{j+1}^X + S_j^Z S_{j+1}^Y), \\ f'_4 &= 4J^4(S_{j-2}^X S_{j-1}^Z S_j^Z - 2S_{j-1}^X S_j^X S_{j+1}^X - 3S_{j-1}^X S_j^Y S_{j+1}^Y - 3S_{j-1}^Y S_j^Y S_{j+1}^X \\ &\quad + S_j^Z S_{j+1}^Z S_{j+2}^X), \text{ etc.} \end{aligned} \tag{3.11}$$

In spite of the basis vectors  $f'_{\nu}$  here are different from the basis vectors  $f_{\nu}$  of the XY case, the relative norms assume the same form, namely,

$$\Delta'_{\nu} = \nu \Delta', \quad \nu = 1, 2, 3, \dots, \tag{3.12}$$

where  $\Delta'_{\nu} = J^2$ . This leads to the same dynamical behavior as with the XY model and the spin Van der Waals model. In particular, the spin correlation function for the TI case is found to be

$$\langle S_j^X(t) S_j^X(0) \rangle = \frac{1}{4} \exp(-\frac{1}{2} J^2 t^2), \tag{3.13}$$

which also agrees with previous results.<sup>4,5</sup> Notice that the basal frequencies  $\Delta'^{\frac{1}{2}}$  and  $\Delta'^{\frac{1}{2}}$  of these models can be made equal by rescaling the coupling constants. Conversely, one can say that the XY model and the TI model are dynamically equivalent with respect to the time evolution of  $S_j^X(t)$ .

Consider now the Brownian analogs of the generalized Langevin equation, Eq.(2.8). The spin random forces for the XY and TI cases are given respectively by

$$F(t) = \sum_{v=1}^{\infty} b_v(t) f_v \quad (3.14a)$$

and

$$F'(t) = \sum_{v=1}^{\infty} b'_v(t) f'_v, \quad (3.14b)$$

with  $f_v$  and  $f'_v$  given by (3.2) and (3.11). The memory functions  $b_v(t)$  can be expressed as

$$b_v(t) = \sum_{m=0}^{\infty} \Delta^{(m-v+1)} c_m^v t^m, \quad (3.15)$$

with a similar expression for  $b'_v(t)$  involving  $\Delta'$ . The coefficients  $c_m^v$  are obtained recursively by

$$\sum_{p=0}^n \sum_{r=0}^{2p} \frac{(-)^{p+r}}{2^p p!} \binom{2p}{r} \frac{1}{2n+v-r} c_{2(n-p)+v-1}^v = \frac{(-)^n}{2^n n! v!}, \quad n=0,1,2,\dots \quad (3.16)$$

The memory function  $\phi(t)$  of the XY model is found to be

$$\phi(t) \equiv b_1(t) = 1 - \frac{2\Delta t^2}{2!} + \frac{10\Delta^2 t^4}{4!} - \frac{74\Delta^3 t^6}{6!} + \frac{706\Delta^4 t^8}{8!} - \frac{8612\Delta^5 t^{10}}{10!} + \dots \quad (3.17)$$

A similar expression for the memory function of the TI model is obtained from Eq.(3.17) by the replacement  $\Delta \rightarrow \Delta'$ . The remaining memory functions  $b_v(t)$  were first calculated by Lee et al<sup>7</sup>, and their results are reproduced here in Fig.2. In that figure,  $\Delta$  is taken to be unity for convenience. From the generalized Langevin equations one can see now that  $S_j^x(t)$  evolves in time modulated by the memory function  $\phi$ . The random force  $F$ , with components along the higher dimensions of the dynamical Hilbert space ( $v = 1 \rightarrow \infty$ ) acts to pull the time evolution away from the basal plane onto higher reaches of  $\Delta$ .

#### IV. CONCLUSIONS

We investigated the time evolution of a tagged spin variable  $S_j^X(t)$  in the one-dimensional  $S=\frac{1}{2}$  isotropic XY model and transverse Ising model at infinite temperature by using the method of recurrence relations. This method lends itself to a detailed description of the dynamical behavior of these systems, whether by looking at the propagation of the excitations along the spin chains, or by examining the effects of the memory functions and the random forces of a generalized Langevin equation. The time evolution of  $S_j^X(t)$  is given as an orthogonal expansion in a properly defined Hilbert space in each of these systems. The relative norms of the basis vectors in each of the XY and TI models have the same structure, resulting in similar dynamical behavior for  $S_j^X(t)$  in both cases. We obtained expressions for the transverse spin correlation functions, relaxation functions, memory functions, and random forces for these systems. These results are valid in the thermodynamic limit ( $N = \infty$ ).

For a finite system, there is always an upper bound for the dimensionality  $d$  of the realized Hilbert space and, as a consequence, only periodic solutions are admissible. In that case the system will eventually return to its initial state with an excitation localized, say, at site  $j$ . Thus, for a finite system, there can never be an equipartition of energy and the system is non-ergodic. On the other hand, for infinite systems the dimensionality of the Hilbert space has no a priori constraints on its upper bound. The dimensionality of the Hilbert space depends on the model as well as on the dynamical variable under consideration.<sup>11</sup>

As we have seen, the Hilbert space of  $S_j^X(t)$  has infinite dimensions in both XY and TI cases discussed here. This leads to a propagation of an excitation throughout the spin chain, whose probability amplitudes decay with time in a Gaussian fashion. The system under consideration never returns to its initial state, thus the process is irreversible. As  $t \rightarrow \infty$ , having an infinite number of basis vectors,  $S_j^X(t)$  must sample all reaches of the Hilbert space and it is ergodic in both the XY and TI models. This conclusion is in accordance with the results of Perk et al<sup>12</sup> for the XY case. In the case where the dynamical variable of interest is a conserved quantity, the dimensionality of its Hilbert space is  $d=1$ , and that variable is non-ergodic. That is the case with the magnetization in the XY model<sup>12,13</sup>. We are currently investigating the formal aspects of the connection between ergodicity and dimensionality of realized dynamical Hilbert spaces. Our results will be reported in a forthcoming paper.

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## FIGURE CAPTIONS

Fig. 1 Probabilities  $A_v^2(t)$  vs time,  $S_j^X(t)$  samples the basis vectors  $f_v$ .  
The time is given in units of the basal frequency  $\Delta^{1/2}$ .

Fig. 2 Memory functions  $b_v(t)$  vs time for both XY and TI models.  
The basal frequencies  $\Delta^{1/2}$  and  $\Delta'^{1/2}$  are taken to be unity in  
both axes.

Fig. 1

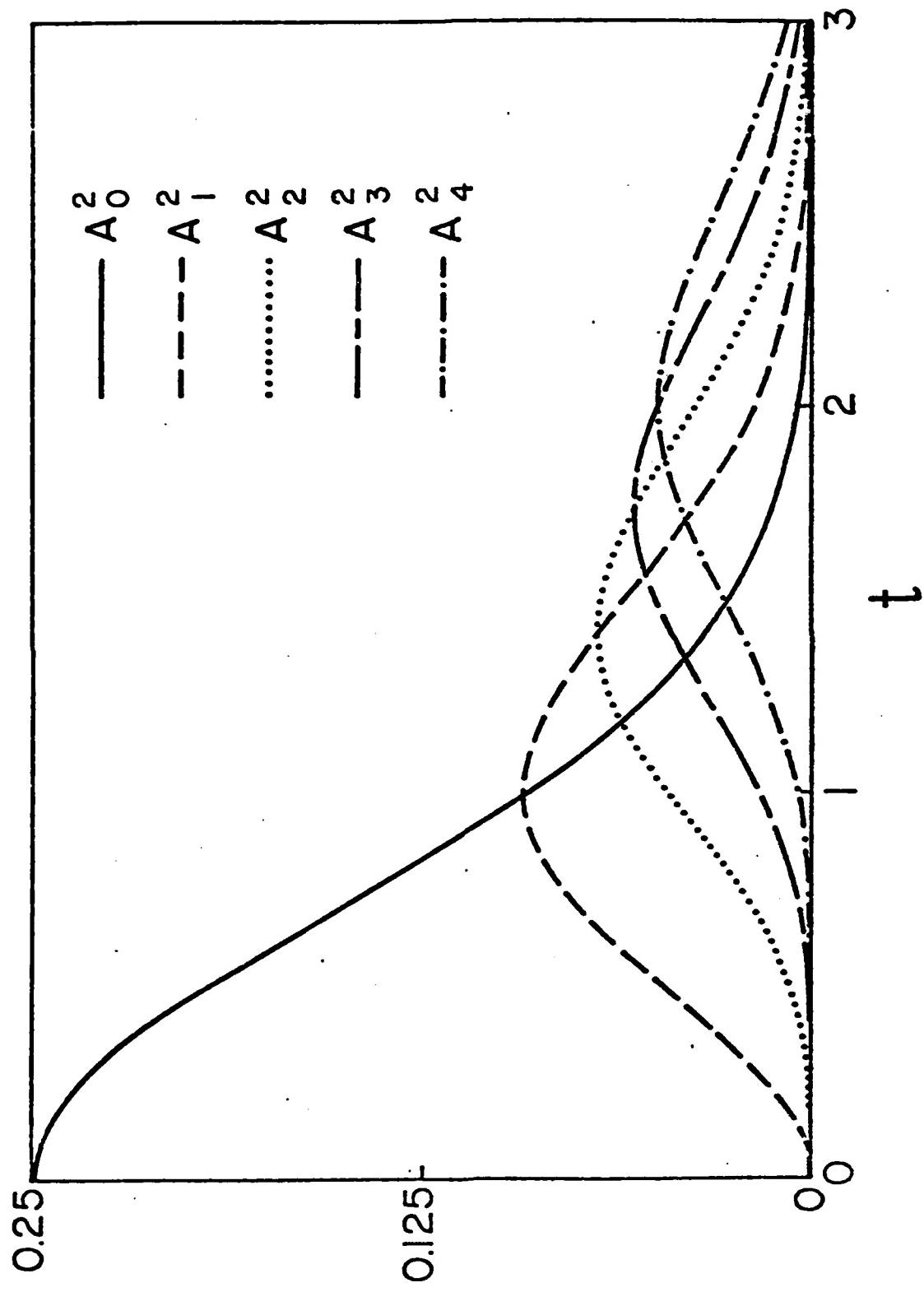
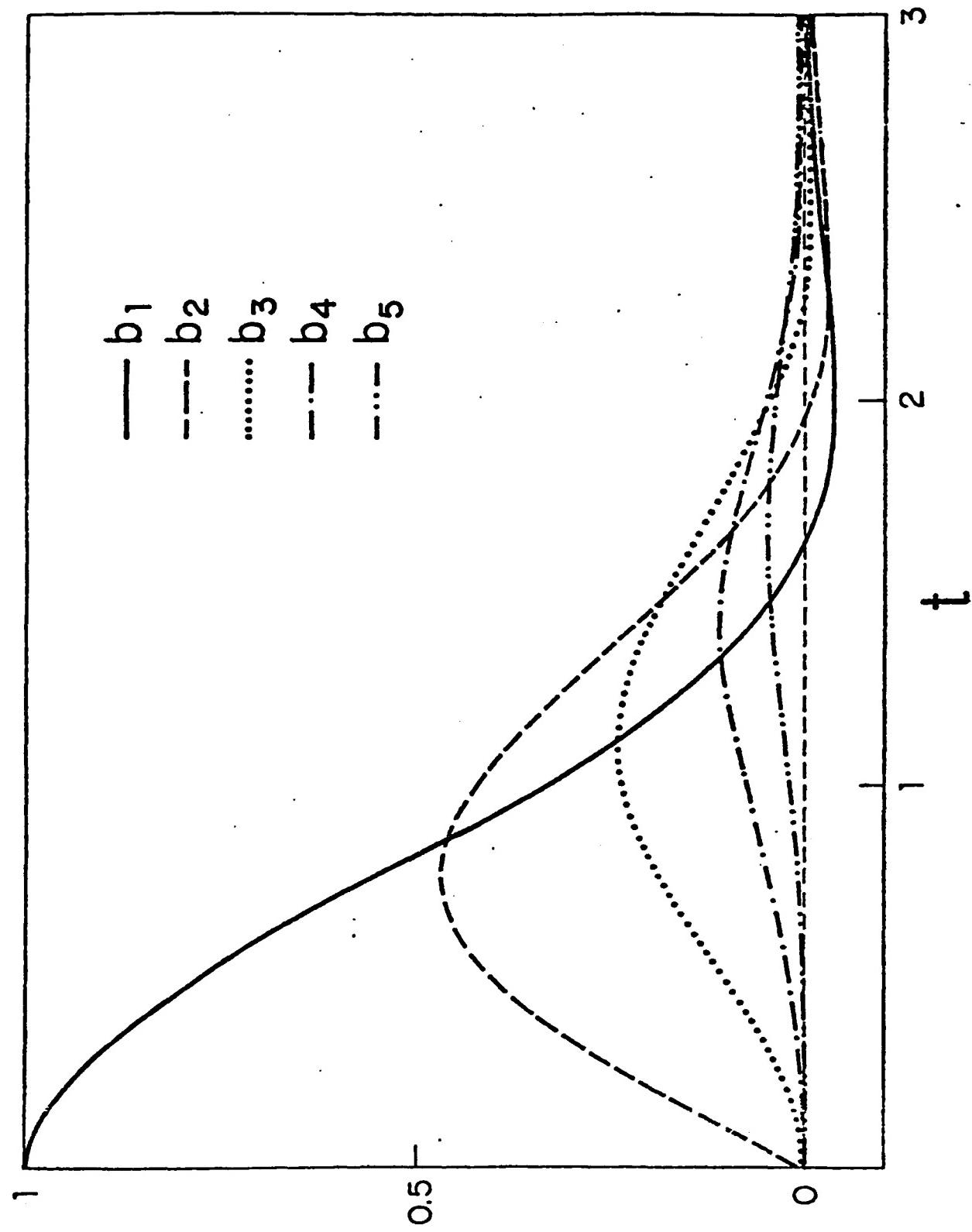


Fig. 2



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D T I C